Theory of the optical properties of segregated (InAs)/(GaSb) superlattices

- Rita Magri

  Dipartimento di Fisica and INFM

  Università di MO e RE, Modena,

  Italy

- Alex Zunger

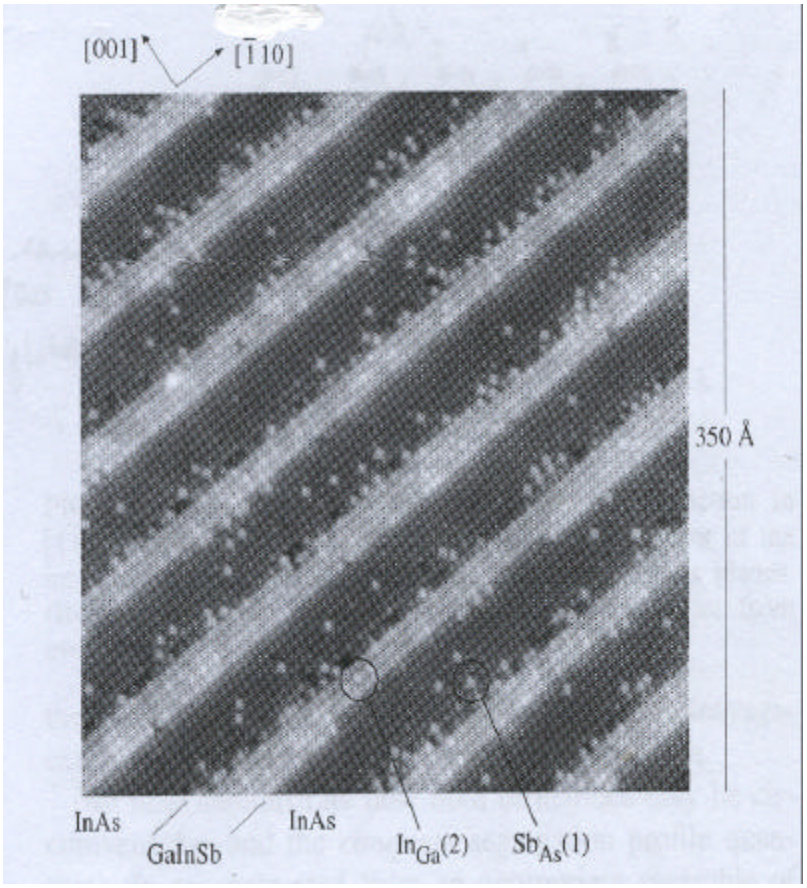
  NREL, Golden, Colorado

  USA

Why to study segregation and interfacial disorder effects?

(for example on the optical spectra)

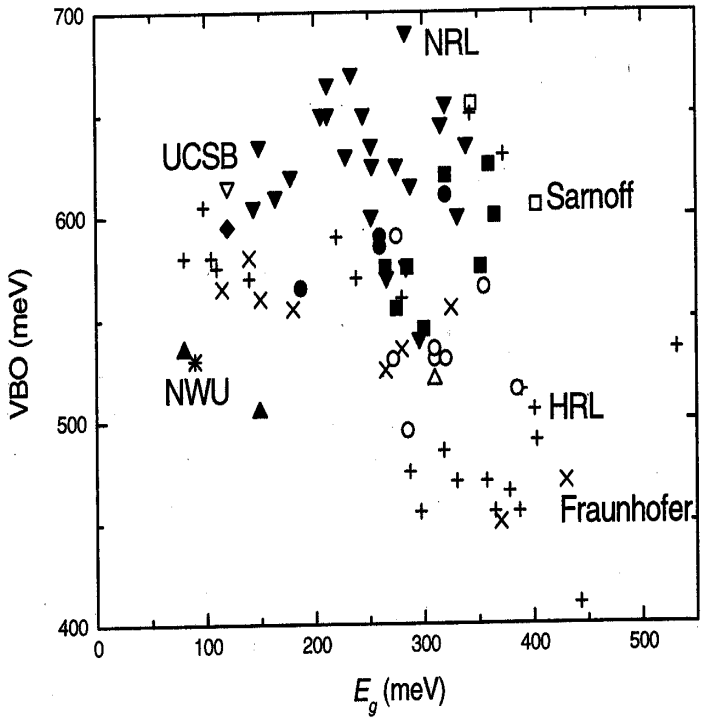
- First Reason: because some deviations from interfacial abruptness are always present in real samples.



(Steinshnider et al. PRL 85,4562 (2000)

- Sb within InAs
- As and In within GaSb
- Interfacial broadening
- Normal (InAs-on-GaSb) IF rougher and more intermixed than inverted IF (Feenstra et al. PRL 72,2749 (1994)
- GaAs-like IF rougher than InSb-like IF (Twigg et al. Philos. Mag. 7,7,(1998)

Possible effects on the gaps of InAs/GaSb SLs and MQWs



- Vurgaftman et al. JAP 89,5815 (2001) fit the measured gaps to 8-band **k·p** theory to extract an average VBO for InAs/GaSb.

• Differences between average offsets derived using data from different groups

• Differences as large as 100 meV for structures that are nominally similar!

Different microscopic morphology (for nominally identical structures) ⟷ <u>Conspicuous</u> differences in gaps

Our EPM

- **SL Symmetry Effects**

  Atomistic approach - we fully solve the single-particle Schrödinger equation where the SL potential is the sum of the atomic screened potentials. This takes into account fully the (D_{2d}or C_{2v}) SL symmetry.

$$V(\underline{r}) = \sum_{na} v_a(|\underline{r} - \underline{R}_{na}|)$$

where

$$v_a(|\underline{r} - \underline{R}_{na}|) = \sum_q e^{iq\bullet(r-R_{na})} v_a(|q|)[1 + dv]$$

and

$$v_a(|q|) = a_0^a \frac{q^2 - a_1^a}{a_2^a e^{a_3^a q^2} - 1}$$

is a continous function of q

- **Environmental Effects**

  Appropriate potentials for the interface bonds In-Sb and Ga-As

  We fit the EPM to:

- experimental gaps
- exptl effective masses
- exptl hydrostatic and biaxial deformation potentials
- LDA-predicted single band edge deformation potentials
- band offsets

of ALL the binary compounds: GaSb, InAs,GaAs and InSb.

Atomic pseudopotentials of Ga in GaSb and in GaAs are different

The potential on each atom is specific of its n.n. environment

$$v_{\mathrm{In}}(\mathrm{As}_n\mathrm{Sb}_{4-n}) = \frac{n}{4} v_{\mathrm{In}}(\mathrm{InAs}) + \frac{4-n}{n} v_{\mathrm{In}}(\mathrm{InSb})$$

- **Strain Effects**

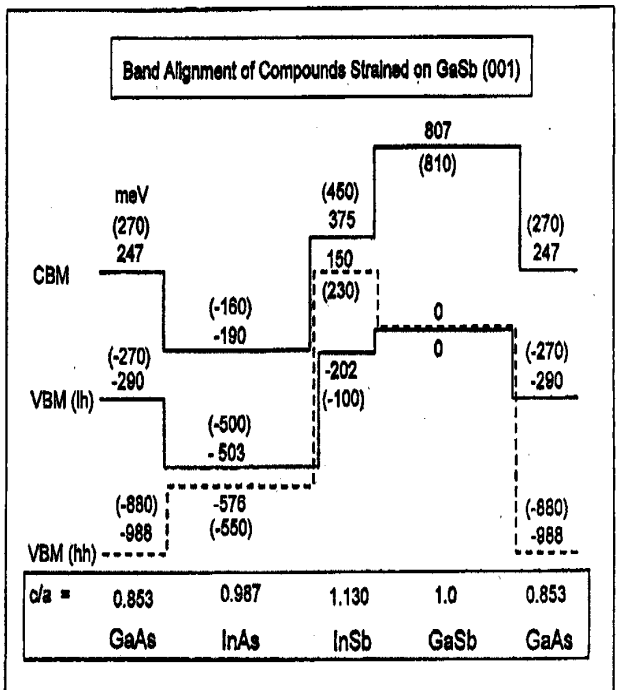
  Our EPM include a parameter fit to the gap and band edge deformation potentials.

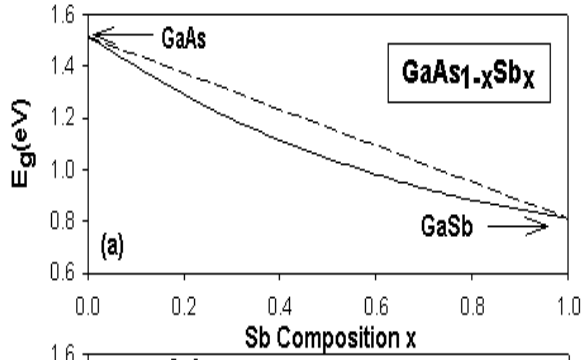
$$dv_{na}(e) = a_4^a \mathrm{Tr}(e)$$

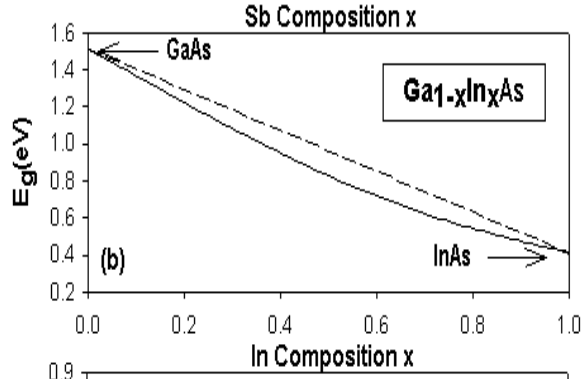
Atomic positions R_{na} in the crystal are locally displaced by a VFF approch

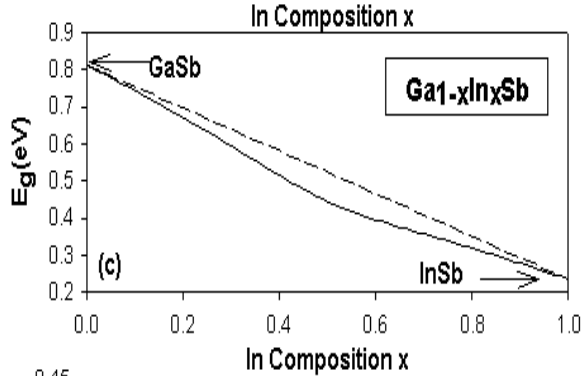
Capabilities of the EPM

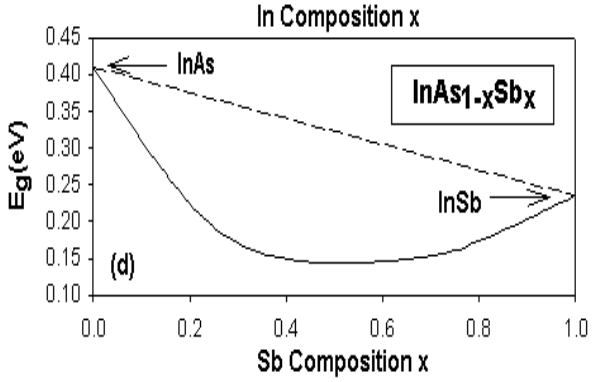
IF specific offsets











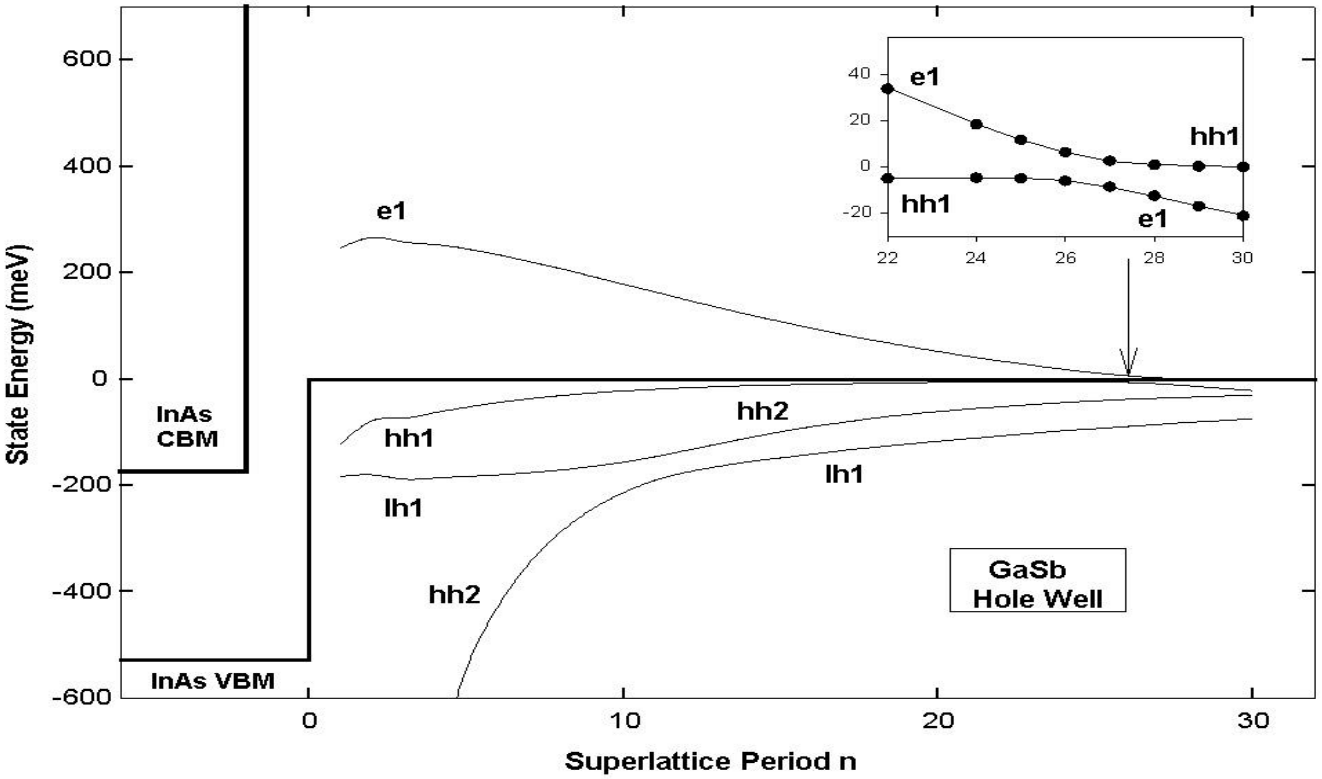
To describe

- IF wavefunction localization
- alloying effects at IF

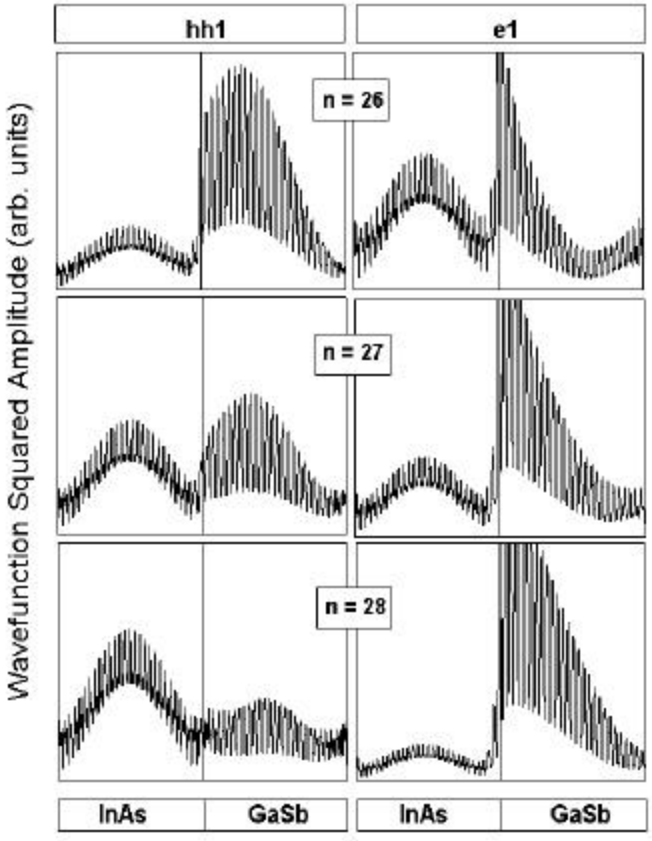
Gap bowing parameters of ternary alloys

Brief summary of the results for the abrupt superlattices

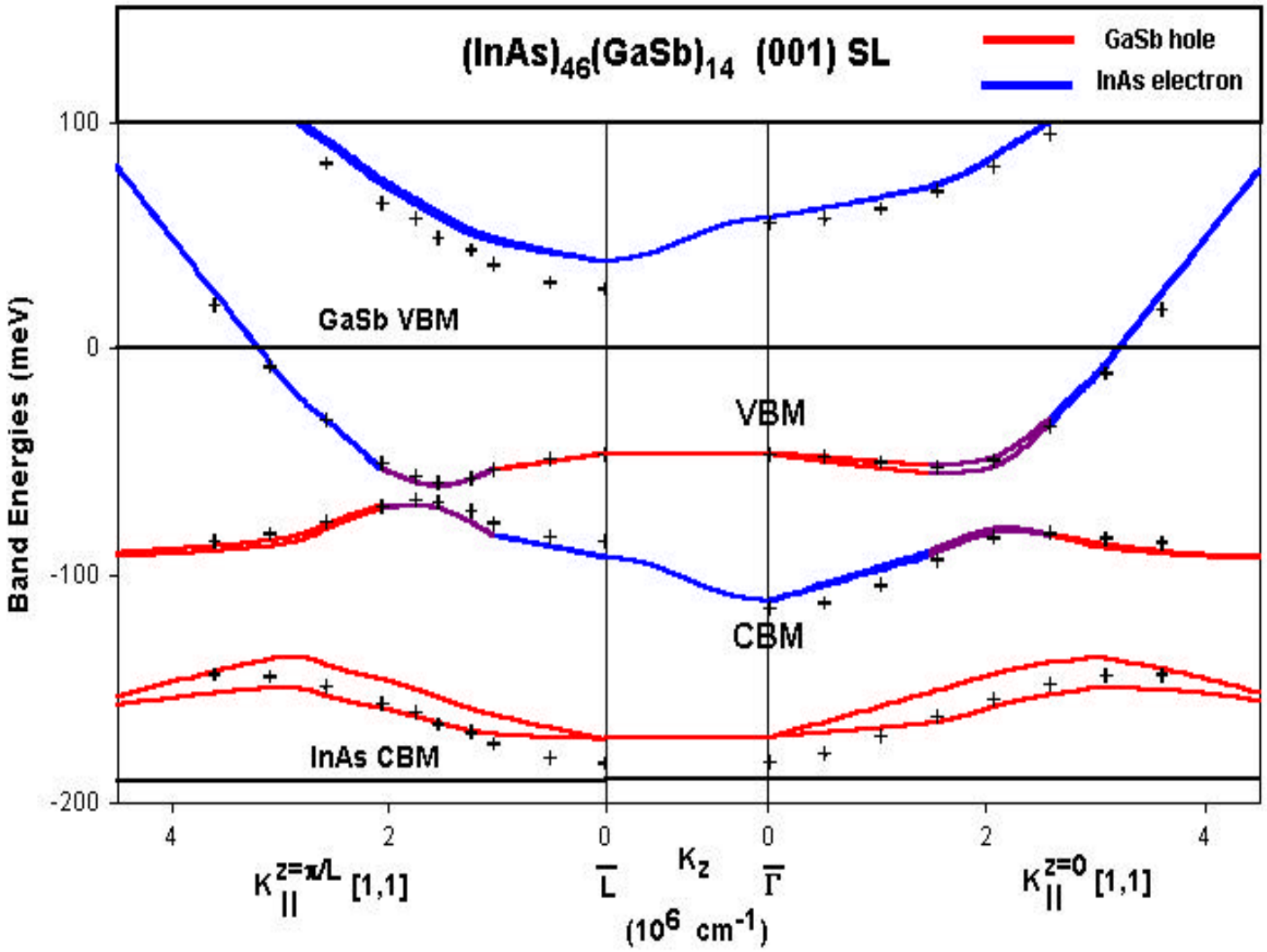
Abrupt $(InAs)_n/(GaSb)_n$ SLs



- Anticrossing period in agreement with experiment



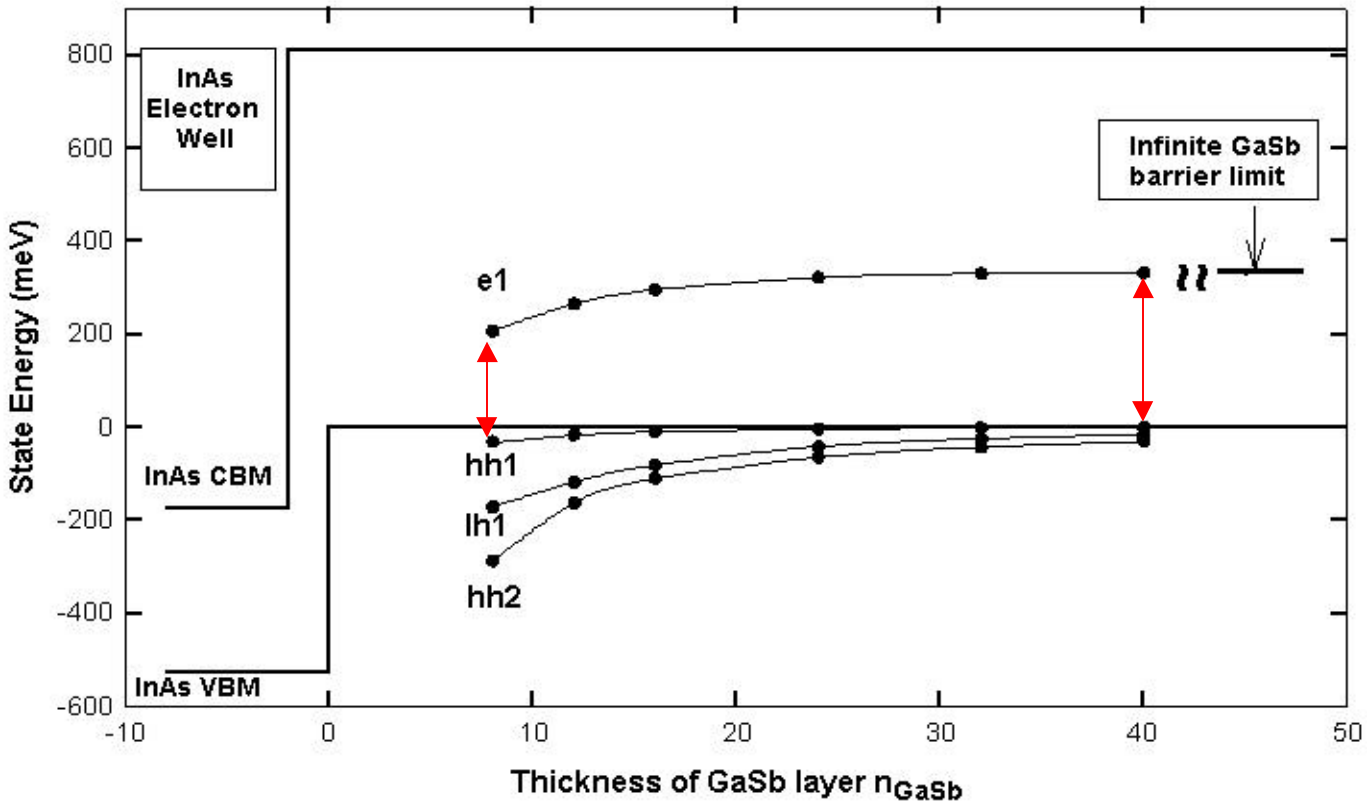
Anticrossing semiconducting band gap



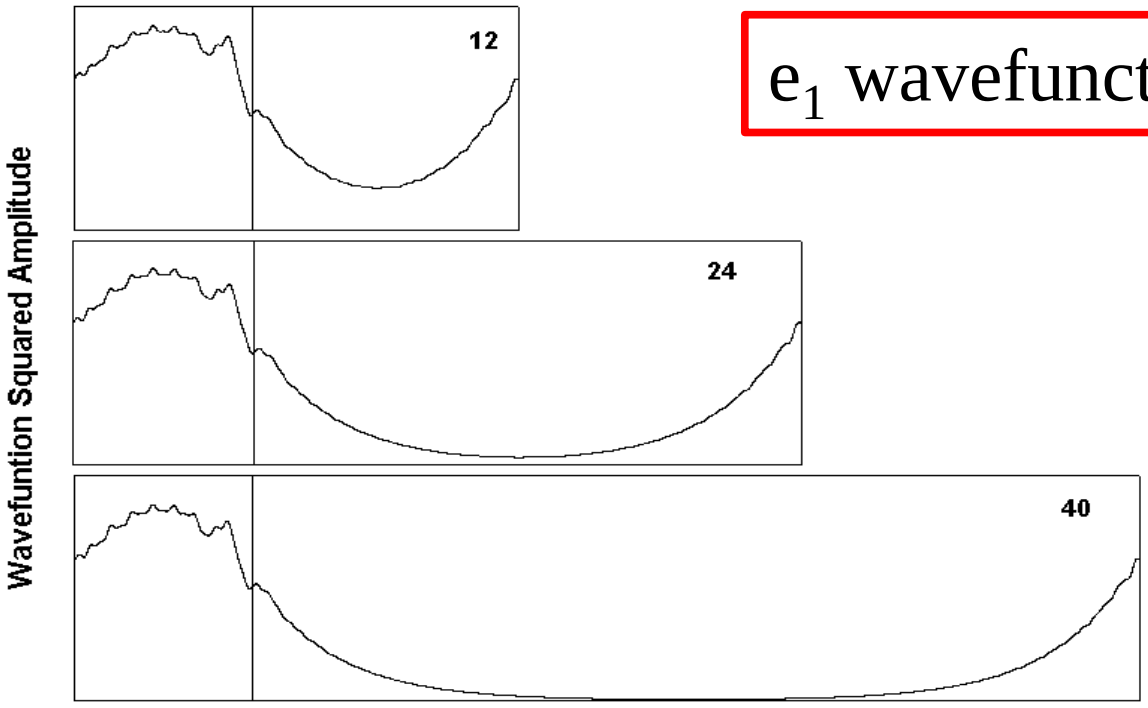
Smaller gap 2-8 meV

- Magri et al., PRB 61,10235 (2000)

Abrupt $(InAs)_8/(GaSb)_n$ SL's

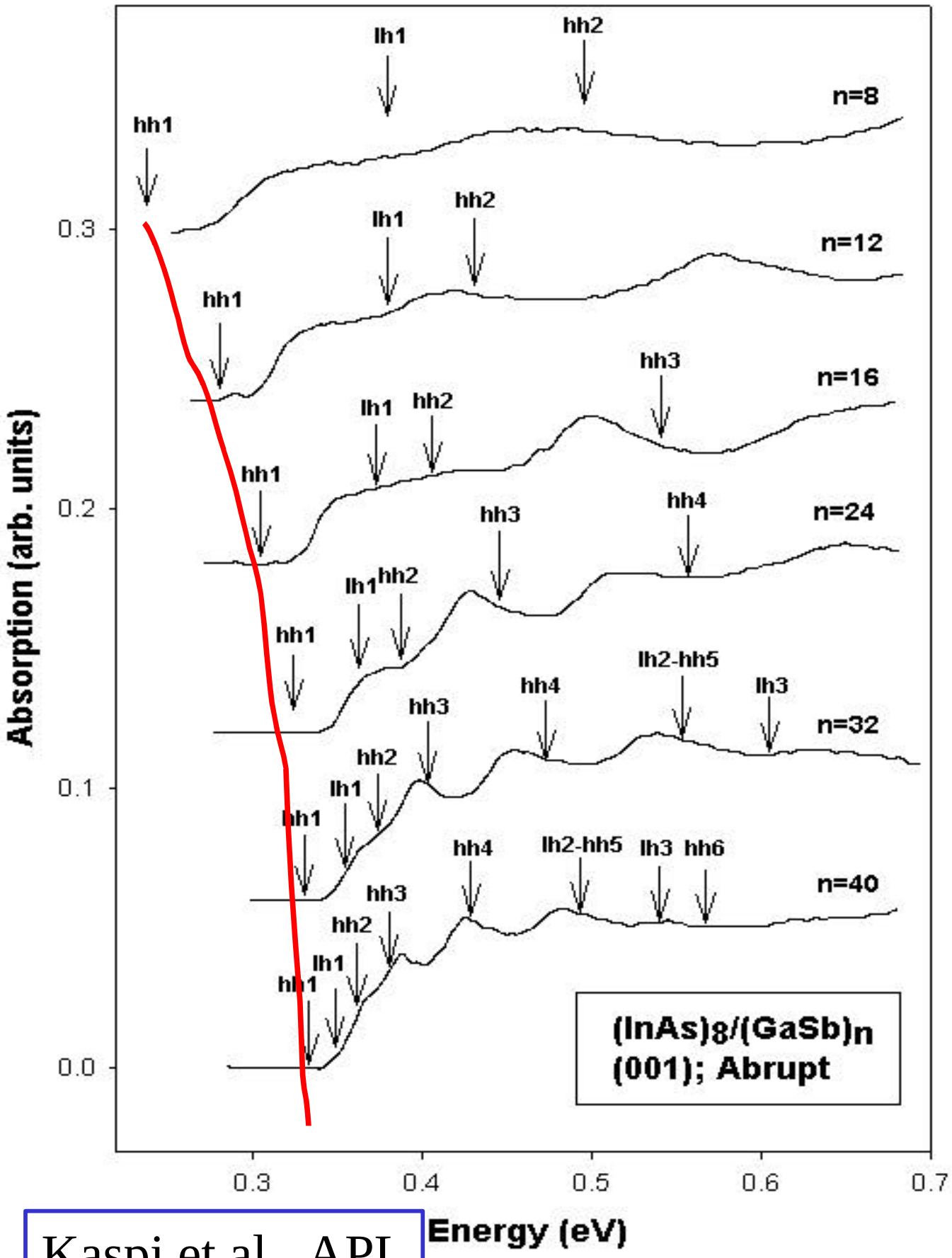


e_1 wavefunction



InAs GaSb

- Arrows - calculated transition energies



Kaspi et al., APL 76, 409 (2000)

Interface Interdiffusion Models

We consider two models:

- **Model I**: The Single-Layer Disorder Model

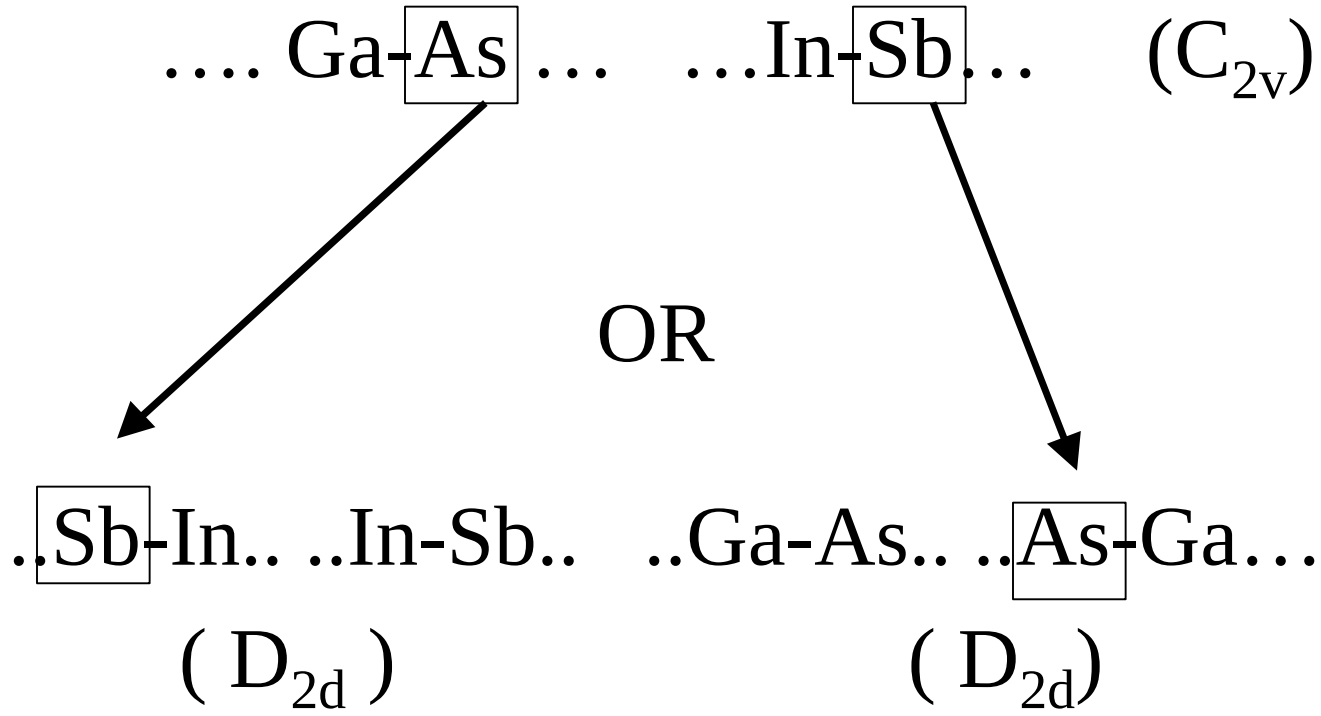
  (to study the effect of the *nature* of the interfacial bonds)

- **Model II**: The Kinetic Model of MBE growth

  (to study the effect of atomic segregation)

Model I: the single-layer model of interfacial disorder

We start from:

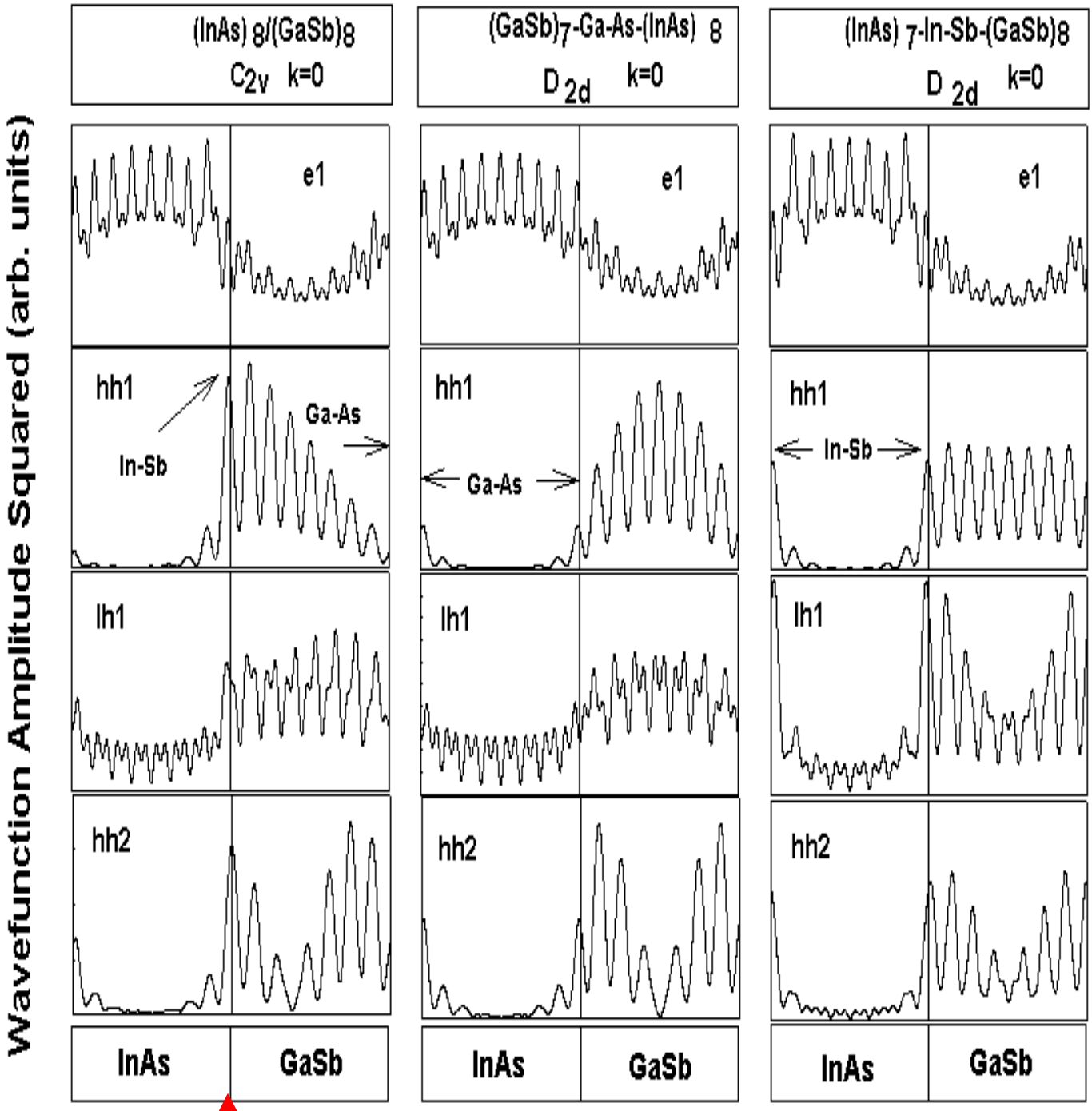


the composition of the interface anion plane is changed CONTINOUSLY

What happens to the electronic structure?

Model I

Electron and hole wavefunctions

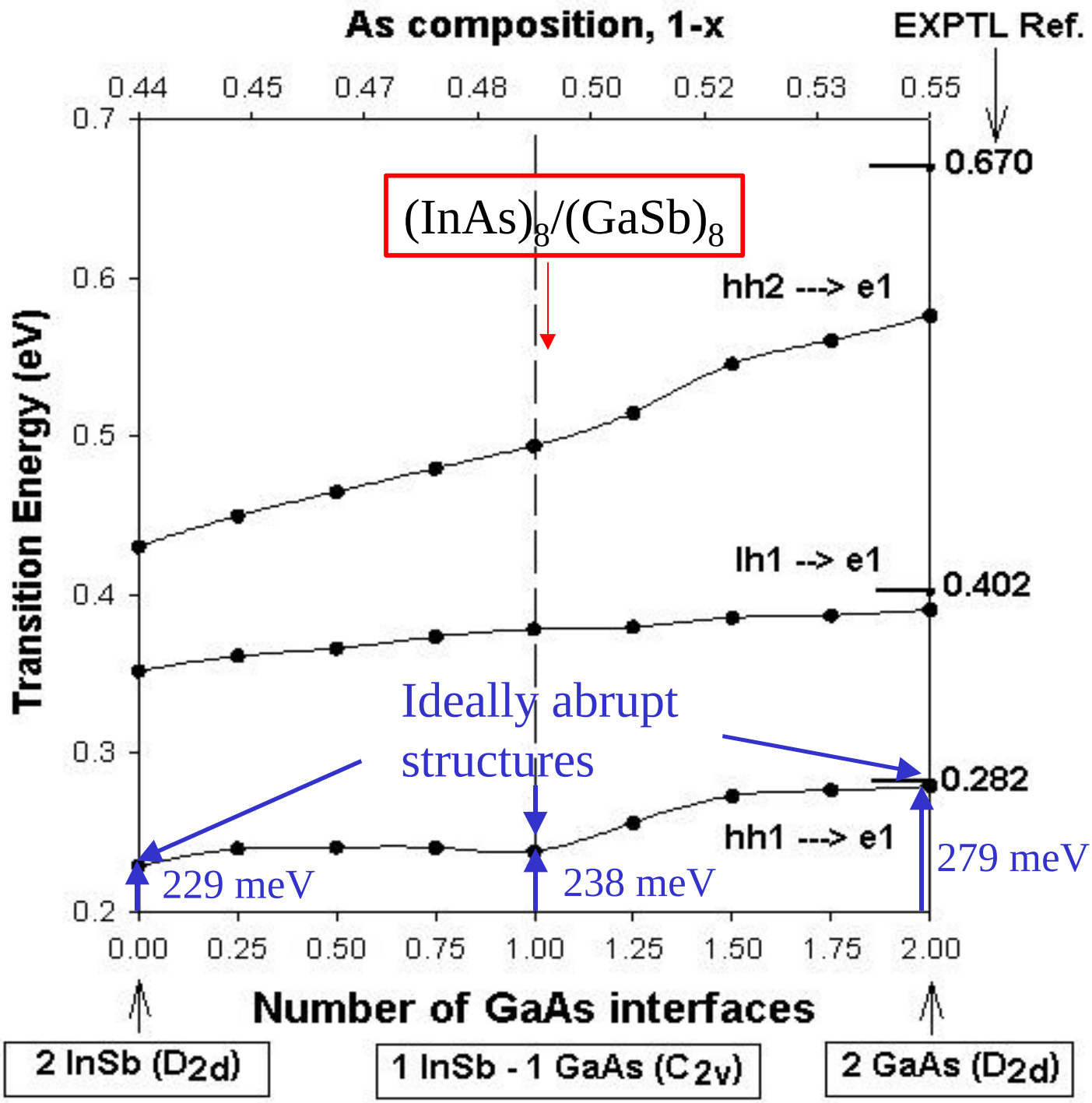


In-Sb IF

- Strong heavy hole localization on In-Sb IF

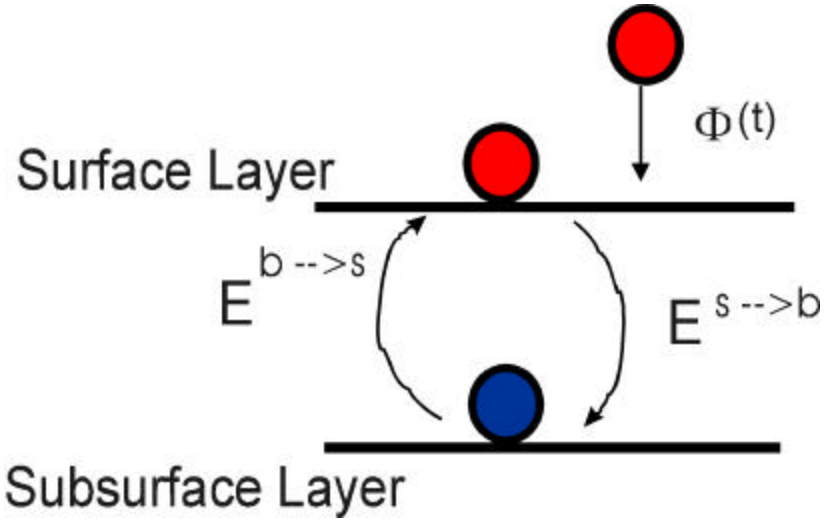
Model I

Interband transition energies



- Gap 50 meV higher for Ga-As interfacial bonds than for In-Sb IF bonds

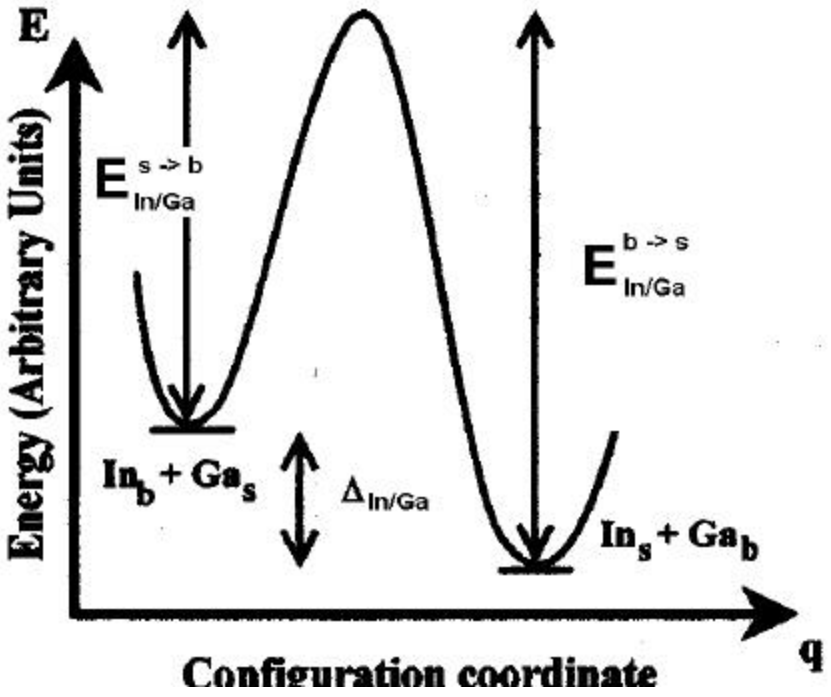
Model II: The kinetic model of MBE growth



- Cations: $E^{b\text{-->}s}_{In/Ga}$ (subsurf In $\leftrightarrow$ surf Ga)
  $E^{s\text{-->}b}_{In/Ga}$ (subsurf Ga $\leftrightarrow$ surf In)
- Anions: $E^{b\text{-->}s}_{Sb/As}$ (subsurf Sb $\leftrightarrow$ surf As)
  $E^{s\text{-->}b}_{Sb/As}$ (subsurf As $\leftrightarrow$ surf Sb)

Segregation Energies:

$\Delta_{In/Ga} = E^{s\text{-->}b}_{In/Ga} - E^{b\text{-->}s}_{In/Ga}$



Model II - The kinetic growth model: the rate equations

- The rates of the exchange reactions depend on the growth temperature T_g

$$P_i = n_i \exp(-E^i_{A/B} / k_B T_g)$$

- The rate of change of the concentration $x_A(t)$ of surface A atoms is:

$$\frac{dx^s_A(t)}{dt} = \Phi_A(t) + P^{b\to s}_{A/B} x^b_A(t) x^s_B(t) - P^{s\to b}_{A/B} x^s_A(t) x^b_B(t)$$

- Under the conditions of the conservation of A atoms, of the total number of atoms and:

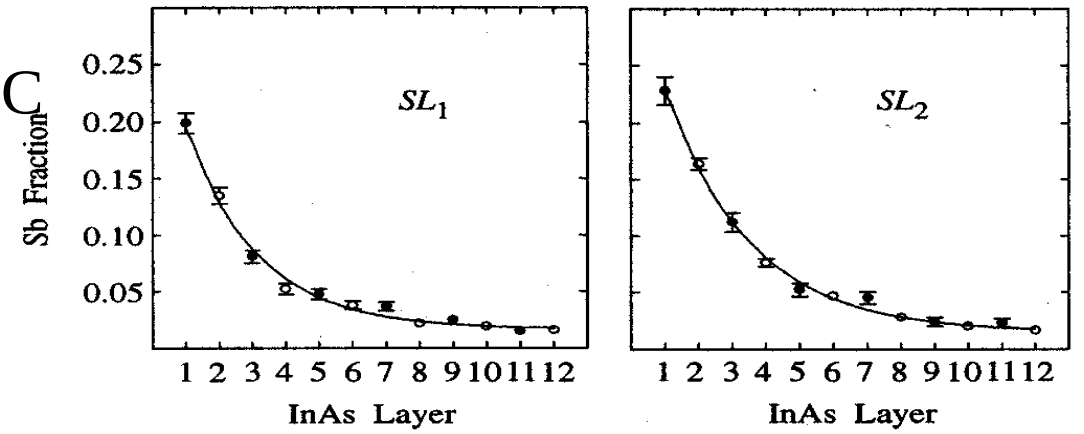
$$x^b_A(t) + x^b_B(t) = 1$$

For cations: $E^{b\text{-->}s}_{In/Ga} = 1.8$ eV , $E^{s\text{-->}b}_{In/Ga} = 2.0$ eV (Dehaese et al. APL 66, 52 (95))

No values in the literature for the anions

The barrier energies for anions

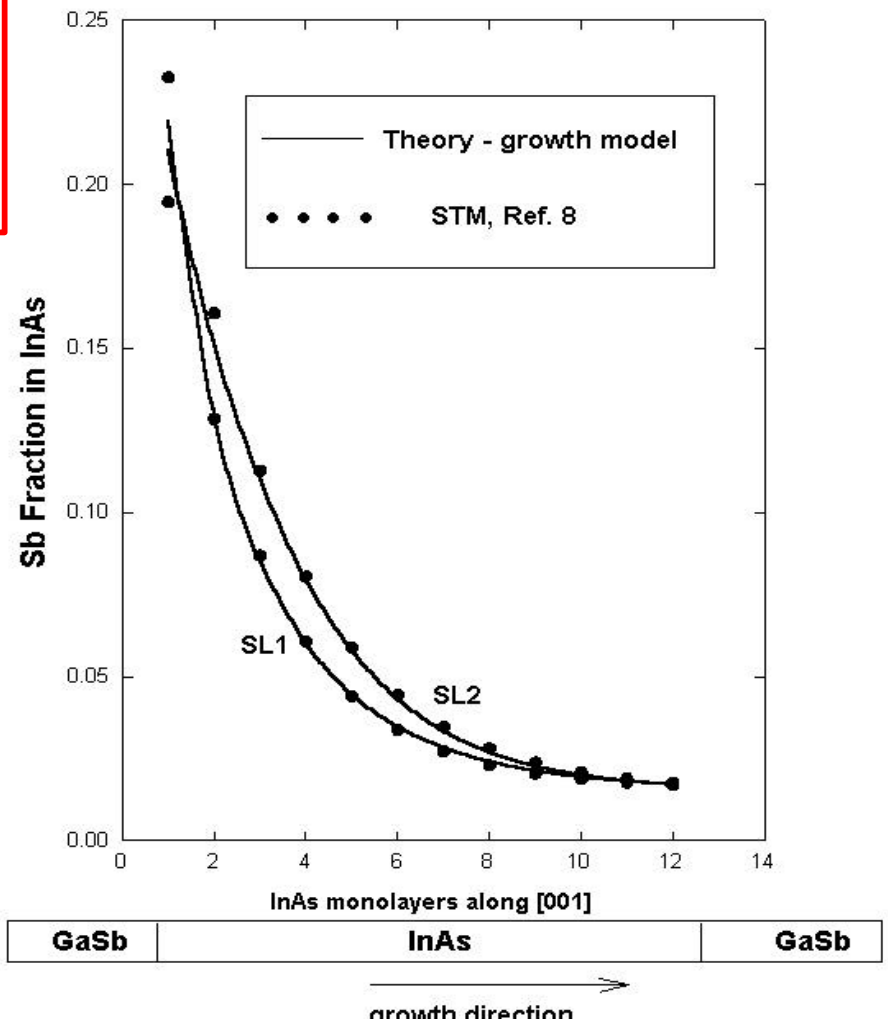
T_g = 380°C



T_g = 440 °C

FIG. 4. Segregation profiles constructed from interleaving even (open symbols) and odd (closed symbols) samplings of the As planes in SL_1 (left) and SL_2 (right). Solid lines are fits to Eq. (1).

Steinshnider et al., PRL 85,4562 (2000)

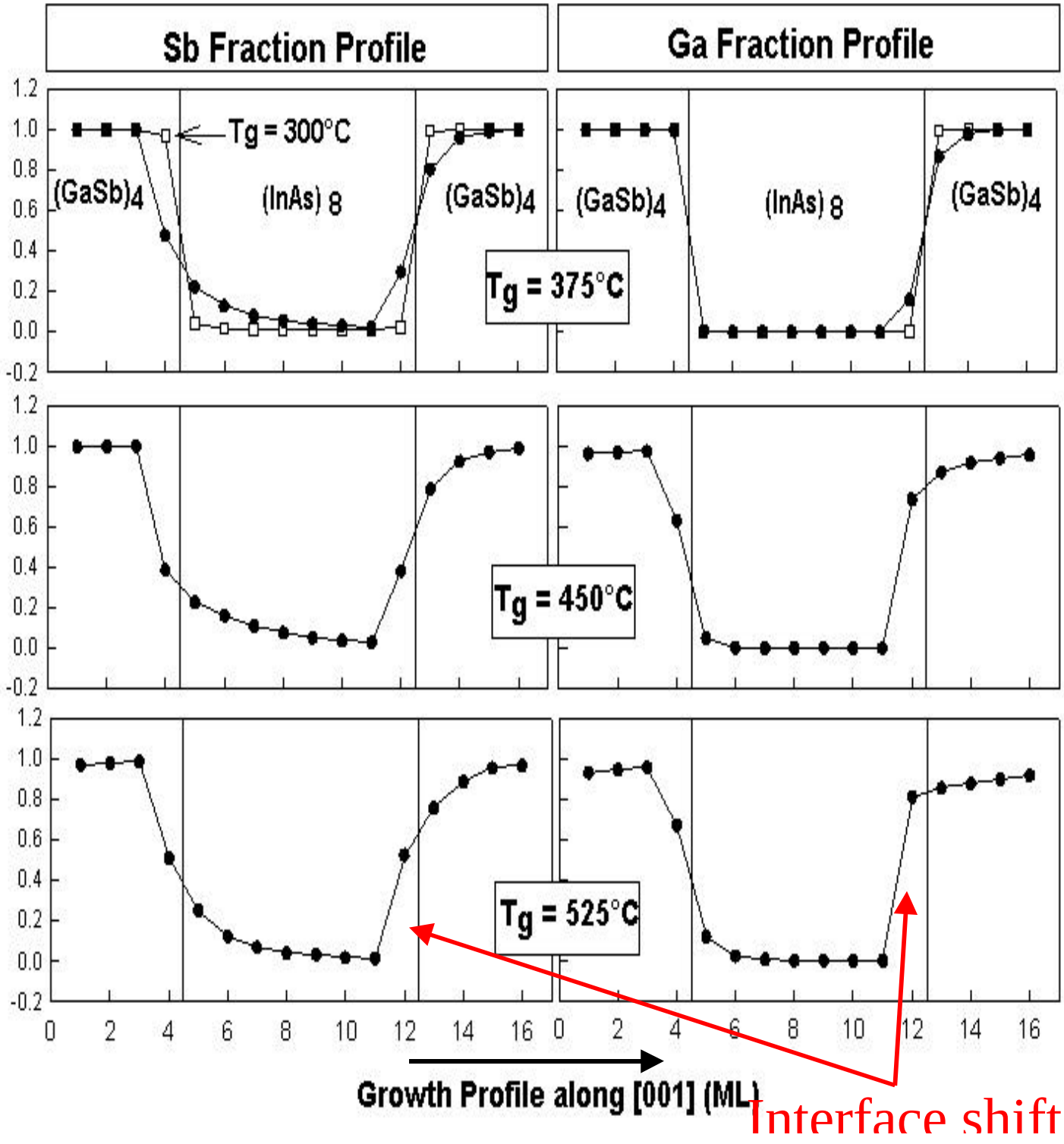


- Fit the growth model to exptl Sb profiles
- $E_{Sb/As}^{b \rightarrow s}$ = 1.68 eV
- $E_{Sb/As}^{s \rightarrow b}$ = 1.75 eV
- r = 0.25 ML/s

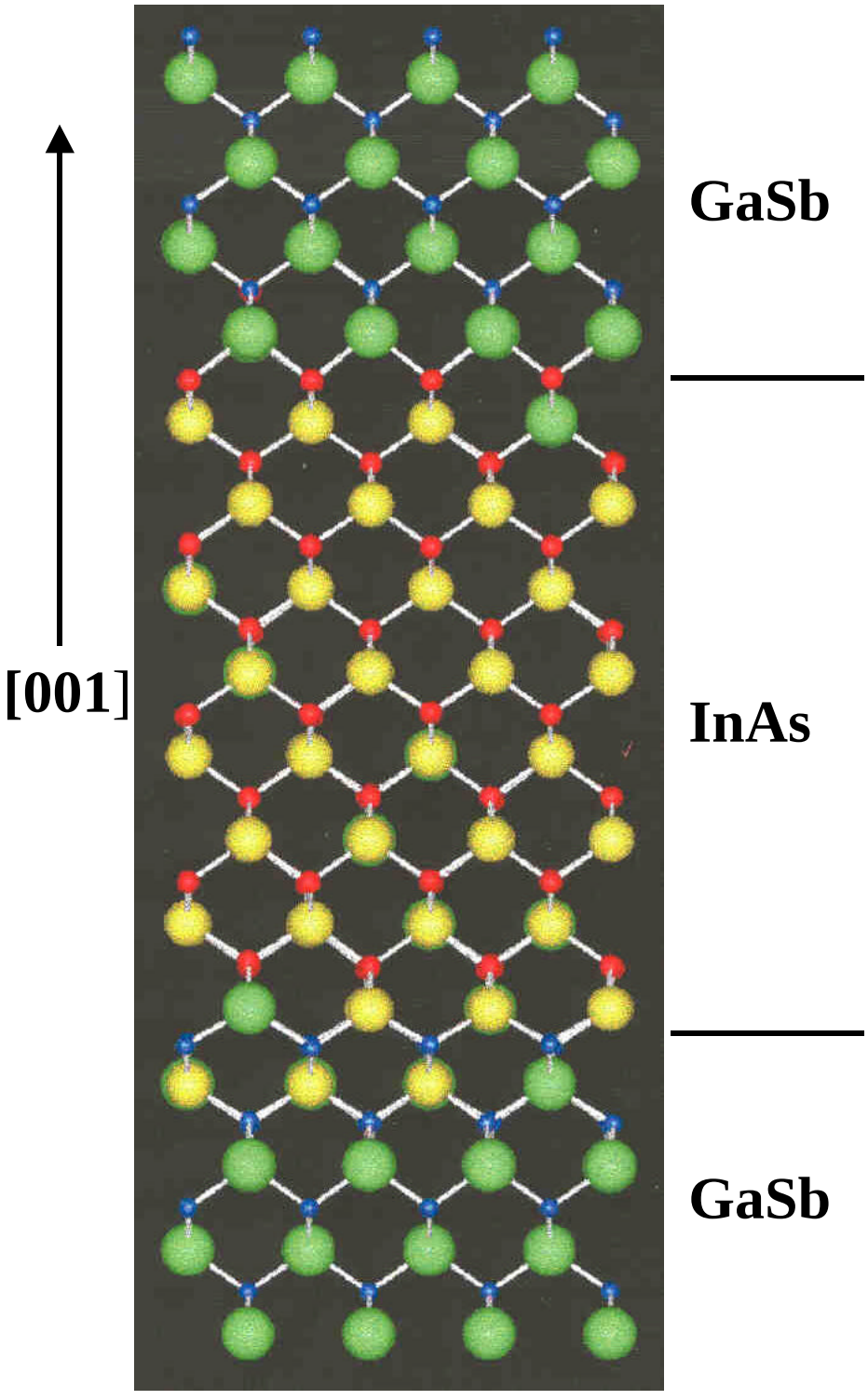
Model II

Superlattice segregation profiles

$(InAs)_8/(GaSb)_8$

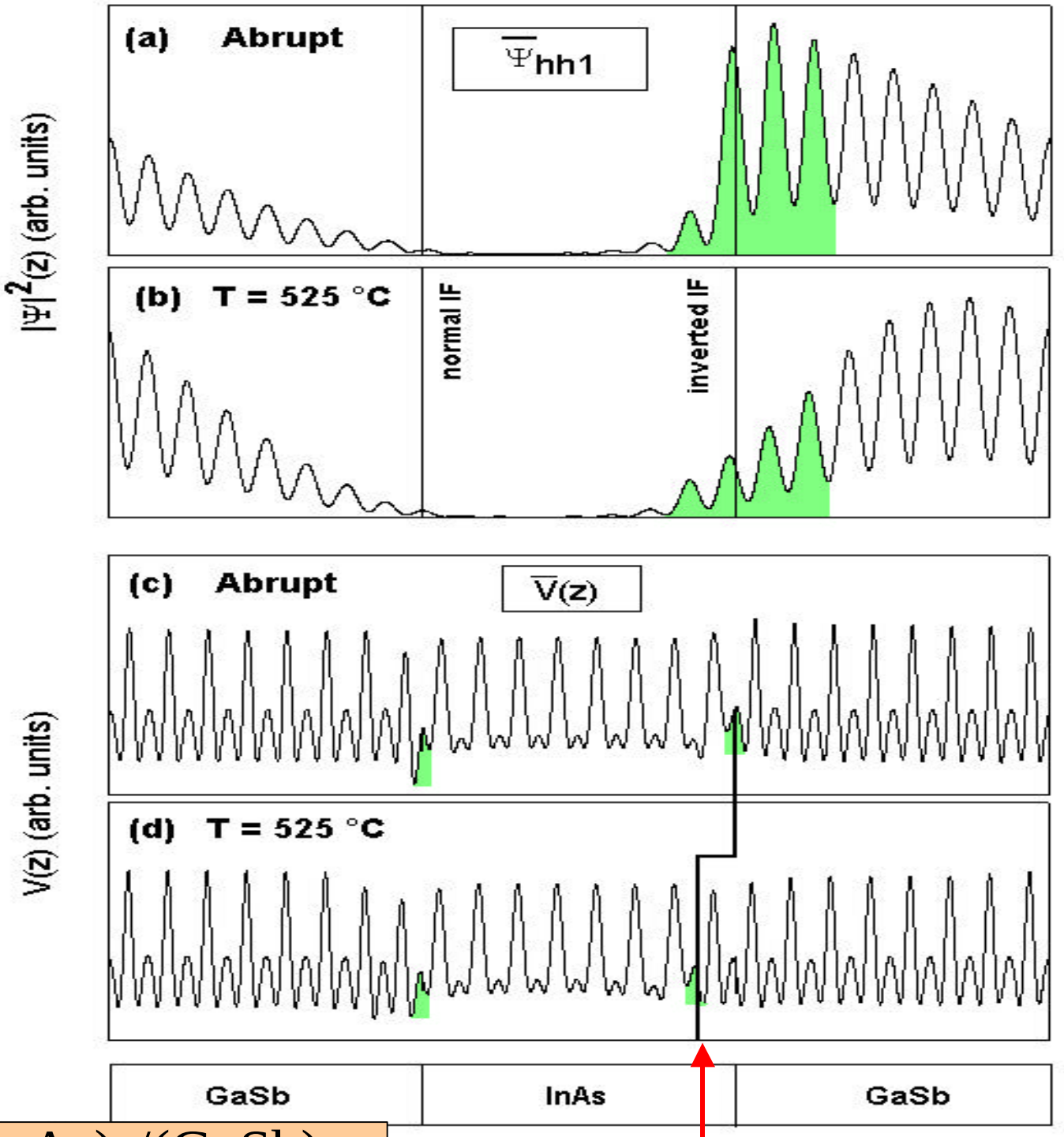


- We assume random atomic arrangements in the (001) planes perpendicular to growth direction consistent with the planar composition profile dictated by the growth model



- Atomic positions in the crystal are locally displaced by a VFF approach

Modification of the heavy hole localization and of the IF potential with segregation



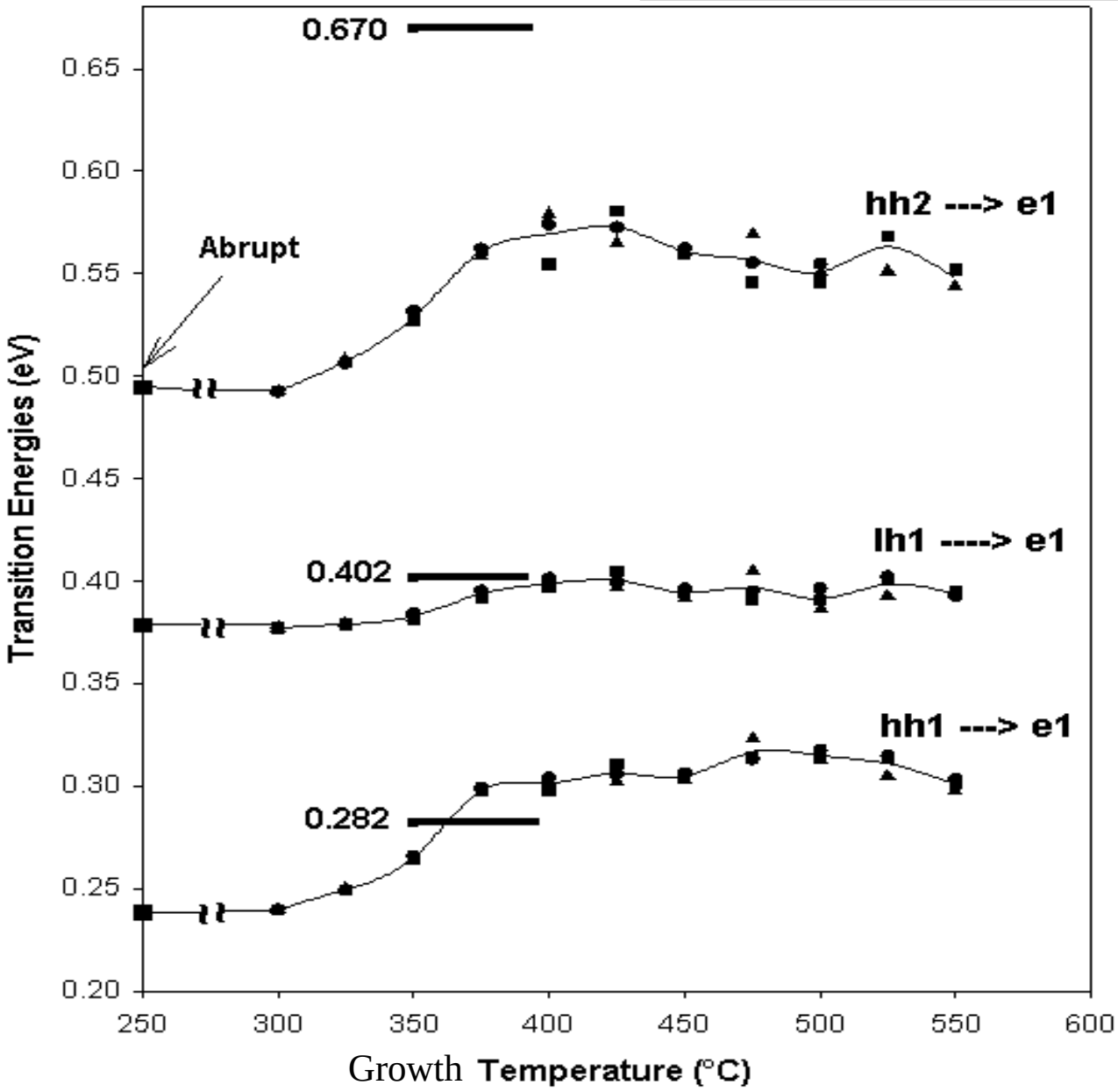
$(InAs)_8/(GaSb)_{16}$

Interface shift

Model II

Effects on transition energies

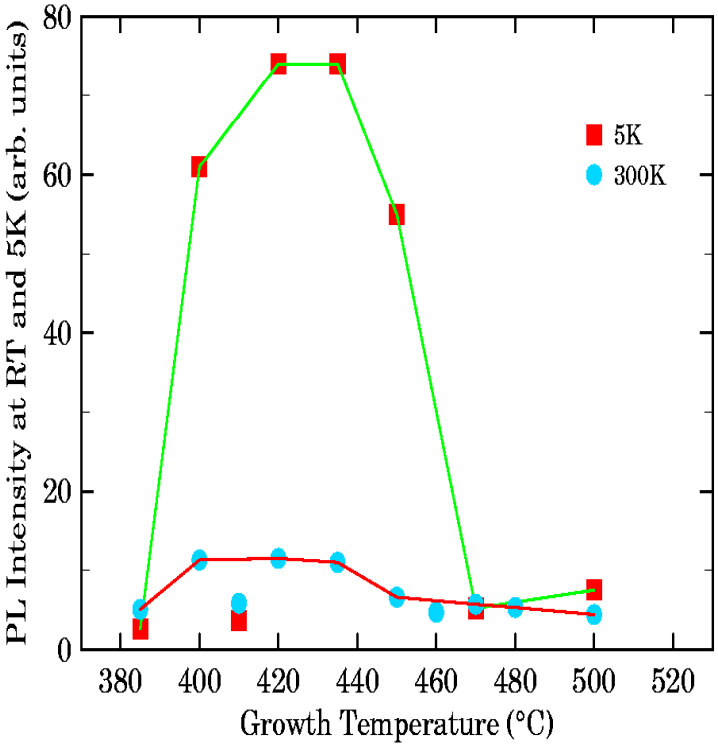
$(InAs)_8/(GaSb)_8$



- Large blue shift of heavy hole - e_1 transitions (50 meV for hh1- e_1)

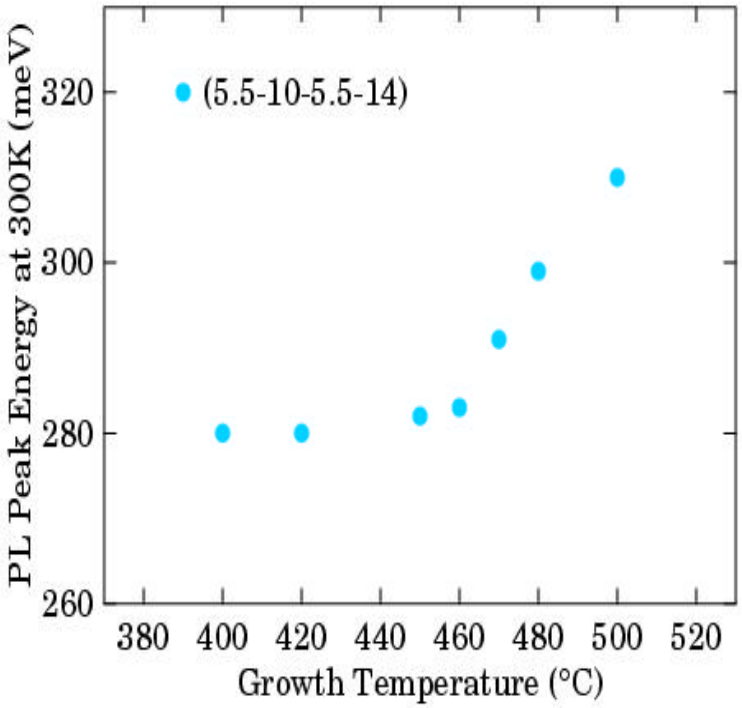
DEPENDENCE ON GROWTH TEMPERATURE

*M. J. Yang, W. J. Moore, B. R. Bennett, and B. V. Shanabrook, Electron. Lett. **34**, 270 (1998)*



PL intensity (laser structures) varies rapidly with growth temperature – Optimal range is 400-450 °C

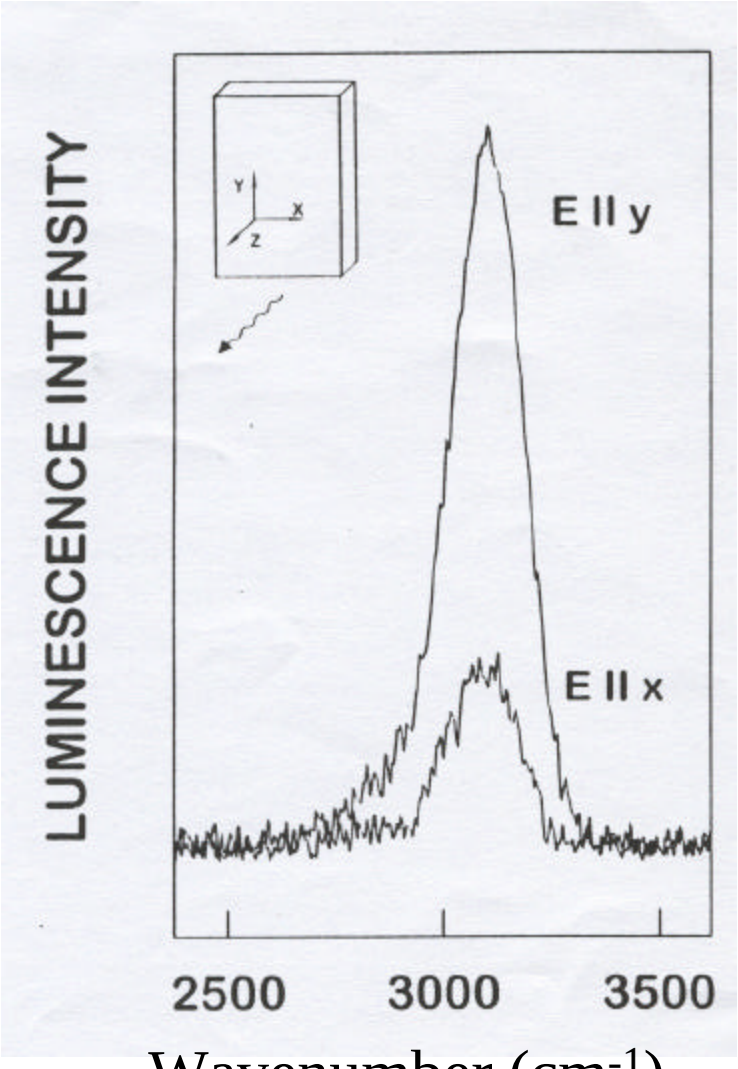
Surprisingly, PL peak (energy gap) also increases significantly with T_{growth} above 450 °C!



In-plane Polarization Anisotropy

When symmetry is C_{2v}:

$$\frac{I^{e\to h}(\vec{p}\|[110])}{I^{e\to h}(\vec{p}\|[\bar{1}10])} \neq 1$$



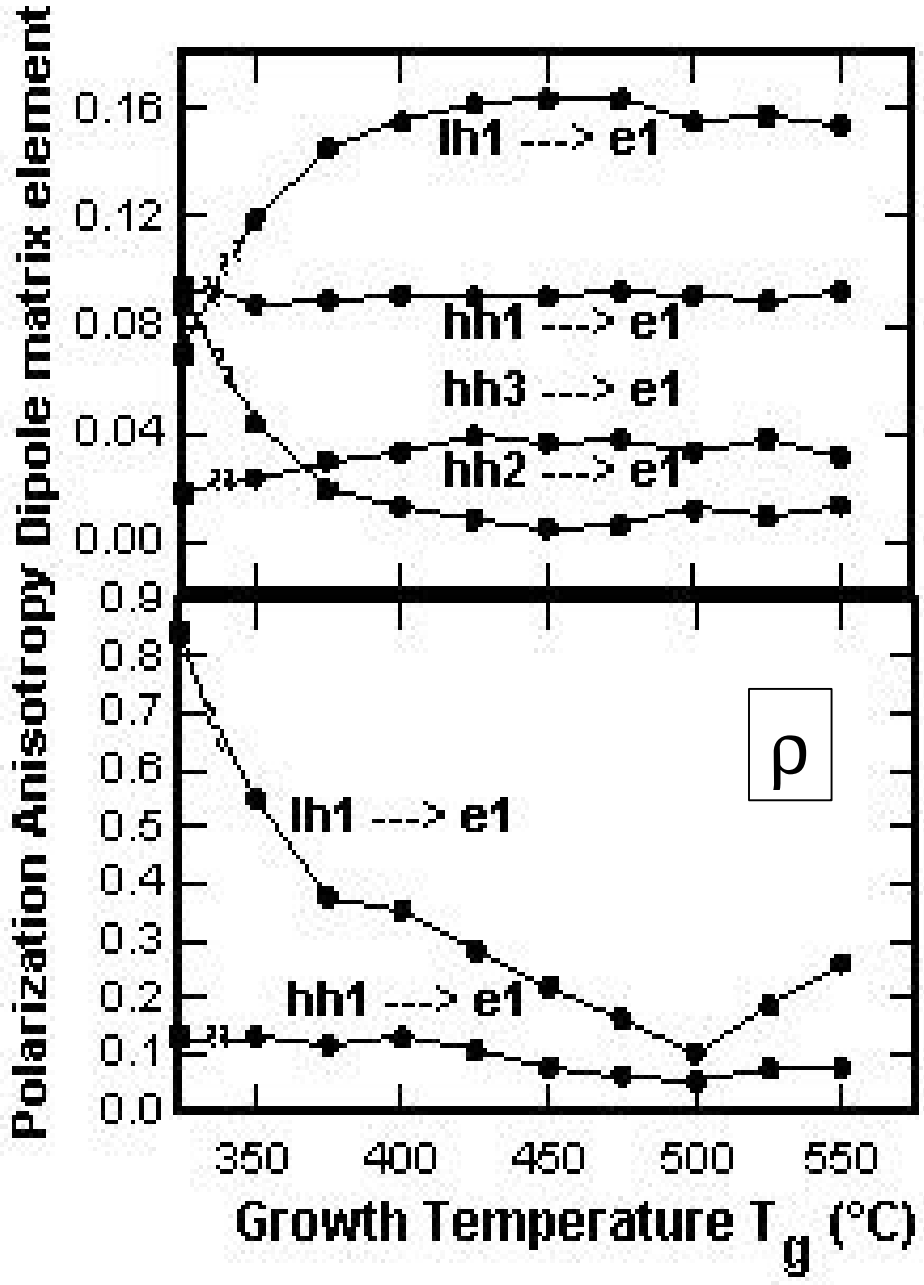
Y=[-110]

X=[110]

InAs/AlSb superlattice

Fuchs et al. in "Antimonide-Related Strained-Layer Heterostructures"

$(InAs)_8/(GaSb)_{16}$



$$r = \frac{\left|P_{110} - P_{-110}\right|}{\left[P_{110} + P_{-110}\right]}$$

- decrease of lh1-hh2 coupling
- decrease of in-plane PA

Summary

- We have modeled interfacial interdiffusion and disorder to study the effects of:

  (1) Interfacial Bonds (Model I)
  (2) Atomic Segregation (Model II)

Results

- Band Gaps are **lower** (50 meV for n = 8 SL's) with InSb Ifs than with GaAs Ifs.
- The **hh1 wavefunction** is strongly l**ocalized** on the In-Sb IF bonds (relative pinning of its energy).
- **Segregation**:

Effects increase with T_g

- Normal IF: anion intermixing and IF broadening
- In penetration into GaSb
- As segregation at the inverted IF

- Segregation causes **blue shifts** of band gaps.

→ • 1 ML narrowing of the InAs well
→ • Reduction of hh1 localization on the InSb IF